COMPETITION OF FERROMAGNETIC AND ANTIFERROMAGNETIC ORDER IN THE SPIN-1/2 XXZ CHAIN AT FINITE TEMPERATURE

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An analytical study is presented of the crossover in the gapless attractive XXZ chain from antiferromagnetic to ferromagnetic behaviour at low to high temperature, respectively. In particular, an analytic formula for the crossover in the long distance asymptotics and explicit results for the nearest-neighbour longitudinal correlation are obtained. We also provide results for the specific heat and magnetic susceptibility for various anisotropies.

1   Introduction

In this paper we pursue the question to which extent the partially anisotropic Heisenberg chain with nearest-neighbour coupling

$$H_{XXZ} = \frac{1}{2} \sum_{j=1}^{L} (\sigma_j^X \sigma_{j+1}^X + \sigma_j^Y \sigma_{j+1}^Y + \Delta \sigma_j^Z \sigma_{j+1}^Z). \tag{1}$$

is described by conformal field theory[1,2]. It is well known that (1) for anisotropy $-1 < \Delta < +1$ has a critical groundstate[3,4,5,6,7], however with quite different physics regarding the elementary excitations[12,13]. There are gapless elementary spin excitations throughout $-1 < \Delta < +1$, but additional bound states in the "attractive" parameter regime $-1 < \Delta < 0$. Note that $\Delta = -1$ corresponds to the isotropic ferromagnetic Heisenberg chain with fully polarized groundstate.

Correlation functions are difficult to calculate, analytical results are known for the nearest-neighbour longitudinal correlation[12] $\langle \sigma_j^Z \sigma_{j+1}^Z \rangle_{T=0}$ (which will be generalized to finite T in Sec. 4) as well as field-theoretical results for the long-range behaviour of correlations for $T = 0$[6,7] and small non-zero T[8,9].

Amazingly, the nearest-neighbour correlation $\langle \sigma_j^Z \sigma_{j+1}^Z \rangle_{T=0}$ is always negative for all anisotropies $-1 < \Delta < +1$. In addition, the longitudinal correlation $\langle \sigma_0^Z \sigma_r^Z \rangle_{T=0}$ for large distances r is negative in the attractive regime.

The finite temperature results for $\langle \sigma_0^Z \sigma_r^Z \rangle$ as found in numerical studies are quite rich [10]. For fixed separation $r \neq 0$ a transition from negative to positive values appears for some temperature $T_0(\Delta, r)$. In [10] the question was raised whether $T_0(\Delta, r)$ possesses a well defined (and non-zero) value in the limit $r \to \infty$. Alternatively, in an asymptotic expansion in exponentials

$$\langle \sigma_0^Z \sigma_r^Z \rangle = A \exp\left(-r/\xi\right) + ..., \tag{2}$$

the temperature dependence of the amplitude A of the dominant term was addressed and it was argued that there is a sign change for some well defined temperature $T_0(\Delta)$ $(= T_0(\Delta, \infty))$. Nothing like this is observed in the "repulsive" regime where correlations show simple antiferromagnetic oscillations.

In the current work we want to understand analytically the sign change phenomenon. In particular, we aim at an analytic formula for T_0, see (28). For two reasons, these questions are not purely academic. First, the "attractive" XXZ chain is often considered as a system with ferromagnetic interactions, however with antiferromagnetic groundstate, i.e. vanishing magnetization. Our analysis is aimed at a resolution of the somewhat unintuitive picture in the way of a crossover from dominant ferromagnetic correlations at high to dominant antiferromagnetic correlations at low temperatures. Second, we address the fundamental problem of the additional energy scale that has to enter the description of the "attractive" regime, but is absent in the "repulsive" case. Naturally, we will be led to pay attention to the existence of bound states.

In Sec. 2 we review the known groundstate properties of the XXZ chain, and in Sec. 3 we set up our formalism for finite temperatures on the basis of the quantum transfer matrix. In Sec. 4 we address the problem of crossover phenomena in correlation functions and macroscopic properties. Finally, in Sec. 5 we summarize our results and list the open problems.

2 Groundstate Properties

In (1) the anisotropy Δ is conveniently parametrized by

$$\Delta = \cos\gamma \tag{3}$$

where the range $0 \leq \gamma \leq \pi/2$ corresponds to repulsive interactions and $\pi/2 \leq \gamma < \pi$ to attractive interactions. The elementary excitations on the (antiferromagnetic) groundstate are free states with dispersion relation

$$\epsilon_f(k) = v \sin k, \qquad 0 \leq k \leq \pi, \tag{4}$$

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and "sound" velocity

$$v = \frac{\sin\gamma}{\gamma}\pi. \tag{5}$$

In addition to these "free states" there occur "bound states" in the attractive regime $\pi/2 \le \gamma < \pi$. Depending on the anisotropy there are different bound states labeled by an integer μ in the range $1 \le \mu \le \left[\frac{\gamma}{\pi-\gamma}\right]$ with dispersion [12,13]

$$\epsilon_b(k) = v\,2\sin\frac{k}{2}\sqrt{1 + a_\mu^2 \sin^2\frac{k}{2}}, \qquad a_\mu = \cot\left(\mu\frac{\pi-\gamma}{\gamma}\frac{\pi}{2}\right). \tag{6}$$

and $0 \le k \le \pi$. Note the same velocity of the bound state dispersion as for the free state dispersion. However, for finite momentum the energy of the bound states is *larger* than that of the free states.

For the field theoretical description of the XXZ chain the occurence of bound states in the attractive regime does not have any fundamental consequences, because of identical velocities of free and bound states in the long-wave limit. Within the bosonization approach the XXZ chain is mapped to a Sine-Gordon model where the interaction term is argued to be infrared irrelevant (resulting in a Gaussian model). In this way correlation functions for $T = 0$ and small $T > 0$ with asymptotic behaviour

$$C_r \sim C\cos(P_0 r)\left(\frac{\frac{\pi}{\beta v}}{\sinh\frac{\pi}{\beta v}r}\right)^{2x}, \tag{7}$$

are derived [8,9]. To our knowledge the breakdown of this picture at higher temperatures in general, and the occurence of a new temperature scale in the attractive regime (with bound states) in particular has not been studied for the Sine-Gordon model.

The scaling dimension x and "lattice momentum" P_0 are generally different for different correlation functions and given by a formula obtained from lattice calculations

$$x = \frac{1-\gamma/\pi}{2}S^2 + \frac{1}{2(1-\gamma/\pi)}m^2 + k, \qquad P_0 = (S-m)\pi, \tag{8}$$

where S, m, k are integers corresponding to spin, lattice momentum and position in the conformal tower. For the longitudinal spin-spin correlation function the selection rules enforce $S = 0$, but leave open the values for m and k. A simple inspection shows that $(m,k) = (1,0) \;(= (0,1))$ gives the smallest scaling dimension x for the repulsive (attractive) regime.

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3 Finite Temperatures

3.1 Quantum Transfer Matrix

For a treatment of finite temperatures we employ a convenient transfer matrix approach [11,14,15,16]. To this end the quantum chain at finite temperature is mapped via a Trotter-Suzuki decomposition onto a two-dimensional classical model on a square lattice of width L (= chain length) and height N (= Trotter number) and staggered interactions. The free energy and the decay of static correlation functions is completely described by the largest eigenvalue ($\ln \Lambda_0$) and the next-largest eigenvalues ($\ln \Lambda_i$) of the column-to-column transfer matrix

$$
\begin{aligned}
f &= -\frac{1}{\beta} \lim \ln \Lambda_0 \\
C_r &= A_1 \left(\frac{\Lambda_1}{\Lambda_0} \right)^r + A_2 \left(\frac{\Lambda_2}{\Lambda_0} \right)^r + ...
\end{aligned}
\tag{9}
$$

In the limit $N \to \infty$ this matrix is referred to as the quantum transfer matrix (QTM) being the closest analogue to the usual transfer matrix of classical spin chains.

For the XXZ chain integrability is manifest at the level of the QTM in the following way. There is a commuting family of matrices $T(x)$ generated by the spectral parameter x. The QTM is identical to $T(0)$. As most of the physical properties are directly given by the logarithm of $T(0)$ we define $\mathcal{H} = -\ln T(0)$. The lowest eigenvalue of $\mathcal{H}$ gives βf where f is the free energy per chain site. Furthermore, the QTM enjoys translational invariance along the vertical axis within the two-dimensional geometry. The corresponding momentum $\mathcal{P}$ operator is generated by $T(x)$ through differentiation. In summary we have

$$
\begin{aligned}
\mathcal{H} &= -\ln T(0), \\
\mathcal{P} &= -i \sin\gamma \frac{d}{dx} \ln T(x)|_{x=0}.
\end{aligned}
\tag{10}
$$

Note the similarity to the integrability structure of the Hamiltonian H and momentum operator P with one important difference. The momentum operator P is given by the row-to-row transfer matrix and H is given by its derivative. Consequentially, we will often observe a formal correspondence $\mathcal{H}, \mathcal{P} \longleftrightarrow iP, iH$. Of course, in a suitable continuum limit this is easily understood as Hamiltonian and momentum operator are evolution operators with respect to orthogonal directions.

Next, we review the already known eigenvalue equations for the operator $T(x)$. The corresponding eigenvalues are denoted by $\Lambda(x)$ from which the

eigenvalues $\mathcal{E}$ and $\mathcal{K}$ for $\mathcal{H}$ and $\mathcal{P}$ are directly obtained

$$
\begin{aligned}
\mathcal{E} &= -\ln \Lambda(0), \\
\mathcal{K} &= -i \sin \gamma \frac{d}{dx} \ln \Lambda(x)|_{x=0},
\end{aligned}
\tag{11}
$$

the latter one taking all integer multiples of $2\pi/\beta$. This discretization of $\mathcal{K}$ naturally entails a discrete spectrum for $\mathcal{E}$.

3.2 Eigenvalues and Non-Linear Integral Equations

The largest eigenvalue is given by [16]

$$
\ln \Lambda(x) = -\beta e_0(x) + \frac{1}{2\gamma} \int_{-\infty}^{\infty} \frac{\ln[A\overline{A}(y)]}{\cosh \frac{\pi}{\gamma}(x-y)} dy.
\tag{12}
$$

where e_0 is the groundstate energy and $A = 1 + a$, $\overline{A} = 1 + \overline{a}$ are solutions to the following set of non-linear integral equations (NLIE)

$$
\begin{aligned}
\ln a(x) &= -\frac{\beta v}{\cosh \frac{\pi}{\gamma} x} + \frac{\pi}{2(\pi - \gamma)} \beta h \\
&\quad + \int_{-\infty}^{\infty} \left[k(x-y) \ln A(y) - k(x - y - i\gamma + i\epsilon) \ln \overline{A}(y) \right] dy.
\end{aligned}
\tag{13}
$$

h is the externally applied magnetic field and the integration kernel is given by

$$
k(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sinh \left(\frac{\pi}{2} - \gamma \right) k \cos(kx)}{2 \cosh \frac{\gamma}{2} k \sinh \frac{\pi - \gamma}{2} k} dk.
\tag{14}
$$

The corresponding equation for $\overline{a}$ is obtained from Eq. (13) by exchanging $i \to -i$, $h \to -h$ and $a, A \leftrightarrow \overline{a}, \overline{A}$. These equations will be studied numerically in the next section yielding results for the specific heat, magnetic susceptibilities, and nearest-neighbour correlation for various anisotropies Δ and wide temperature ranges.

The next-largest eigenvalues describing the decay of longitudinal spin-spin correlation functions, i.e. eigenvalues with spin quantum number $S = 0$, are given by [16,18]

$$
\begin{aligned}
\ln \Lambda(x) &= -\beta e_0(x) + \ln \left[\tanh \frac{\pi}{2\gamma}(x - \theta_1) \tanh \frac{\pi}{2\gamma}(x - \theta_2) \right] \\
&\quad + \frac{1}{2\gamma} \int_{\infty}^{\infty} \frac{\ln[A\overline{A}(y)]dy}{\cosh \frac{\pi}{\gamma}(x-y)},
\end{aligned}
\tag{15}
$$

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where A and $\overline{A}$ are determined from

$$
\begin{aligned}
\ln a(x) = {} & -\frac{\beta v}{\cosh \frac{\pi}{\gamma} x} + \pi i + \frac{\pi}{2(\pi - \gamma)} \beta h + \ln \frac{\sinh \frac{\pi}{\pi - \gamma}(x - (y_0 + i\gamma/2))}{\sinh \frac{\pi}{\pi - \gamma}(x - (y_0 - i\gamma/2))} \\
& - K(x - (\theta_1 + i\gamma/2)) - K(x - (\theta_2 + i\gamma/2)) \\
& + \int_{\infty}^{\infty} \left[k(x - y) \ln A(y) - k(x - y - i\gamma + i\epsilon) \ln \overline{A}(y) \right] dy. \quad (16)
\end{aligned}
$$

and $K(x)$ is defined by $K(x)' = 2\pi i k(x)$, or explicitly

$$
K(x) = i \int_{-\infty}^{\infty} \frac{\sinh \left(\frac{\pi}{2} - \gamma \right) k \sin(kx)}{2k \cosh \frac{\gamma}{2} k \sinh \frac{\pi - \gamma}{2} k} dk. \quad (17)
$$

There appear three parameters θ_1, θ_2, and y_0 in the upper equations corresponding to "hole positions" (both $\theta_{1,2}$ on the real axis, or forming a complex conjugate pair) and one "complex rapidity" (with $\operatorname{Im}(y_0) = \pi/2$) of the underlying Bethe ansatz pattern for the QTM. There are higher-lying states satisfying similar integral equations, however with more parameters θ_i and y_j.

The parameters θ_1, θ_2, and y_0 do not take arbitrary (continuous) values, they have to satisfy the coupled equations

$$
a(\theta_1 + i\gamma/2) = a(\theta_2 + i\gamma/2) = a(y_0 + i\gamma/2) = -1, \quad (18)
$$

leading to a quantization of the eigenvalues. In general the equations (16,18) have to be solved numerically in order to deal with the problem of non-linearity. For the case of the largest and next-largest eigenvalues an iterative approach proved useful showing convergence within a numerical accuracy of 10^{-6} already after approx. 10 steps, see ref. [16] for the non-critical cases with $\Delta > 1$ and $\Delta < -1$, and ref. [17] for the critical case $\Delta = 1$. A comparable numerical analysis for $-1 < \Delta < 1$ is in progress, however not yet completed. For this reason we apply an analytical study within a reasonable approximation to (16,18).

3.3 Conformal Field Limit for Low Temperatures

In [16] the equations (15,16) were treated in the low-temperature limit. Despite the apparent complexity of the non-linear integral equations, quite a universal picture evolved. A certain symmetry of the integration kernel allowed for analytic manipulations avoiding the necessity of an explicit solution of the non-linear equations. Each eigenvalue could be written in terms of dilogarithmic integrals which resulted in the explicit formula

$$
\ln \Lambda = -\beta e_0 - \frac{2\pi}{v} T(x - c/12) + o(T^2) + iP_0, \quad (19)
$$

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where the central charge is $c = 1$ and the scaling dimension x and lattice momentum P_0 are given by (8). From (9,19) we see

$$C_r \sim \cos(P_0 r)\epsilon^{-\frac{2\pi}{v}xTr}. \tag{20}$$

which coincides with the conformal field theory result (7) in the low-temperature limit.

On one hand we see that (15,16) recover CFT, on the other hand, the non-linear integral equations are not restricted to low temperatures, but go beyond. It is this behaviour that will be studied in the next sections.

3.4 Solution in Lowest Order

A principal treatment of the NLIE is based on iterations. For instance in the case of (13) a reasonable initial choice for the functions a and $\overline{a}$ is just $a_0 = \overline{a}_0 = 0$. Inserting this into the right hand side of (13) leads to

$$\ln a_1(x) = -\frac{\beta v}{\cosh \frac{\pi}{\gamma}x}. \tag{21}$$

This process should be continued *ad infinitum*, however we content ourselves with the approximation a_1 for the function a. Inserting a_1 and $\overline{a}_1$ into (12) we obtain the *first order approximation* (1OA) in the sense of an iterative procedure to the largest eigenvalue of the QTM which already reproduces correctly: (i) the low-temperature asymptotics $\ln \Lambda = -\beta e_0 + c(\pi T/6v)$ with central charge $c = 1$, *and* (ii) the high-temperature behaviour $\ln \Lambda = \ln 2$. This success may be understood in the following way. At low temperatures the corrections described by the integral terms in (13) are small, and at high temperatures both of them cancel each other. We conclude that the (1OA) is a respectable approximation useful for the entire temperature range.

Free States

Next, we study the excitations (16,18) in (1OA) yielding

$$\ln \Lambda(x) = \ln \left[\tanh \frac{\pi}{2\gamma}(x - \theta_1) \tanh \frac{\pi}{2\gamma}(x - \theta_2) \right], \tag{22}$$

where we have dropped the common offset $-\beta e_0(x)$ in (15). From this and (11) we derive the eigenvalues

$$\begin{aligned} \mathcal{E} &= \epsilon_1 + \epsilon_2, \\ \mathcal{K} &= \kappa_f(\epsilon_1) + \kappa_f(\epsilon_2), \qquad \kappa_f(\epsilon) = \pm v \sinh \epsilon, \end{aligned} \tag{23}$$

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where the parameters θ_i have been parametrized by $\epsilon_i(\geq 0)$ such that κ_i is a unique function of ϵ_i except for the sign in the κ_f dispersion which is given by the sign of the parameter θ_i. Note the similarity of the "momentum-energy" dispersion $\kappa_f(\epsilon)$ for the "free states" of the QTM with the dispersion (4)

$$\kappa_f(\epsilon) = -i\epsilon_f(i\epsilon). \tag{24}$$

We know already from general principles that $\mathcal{K}$ is strictly equal to an integer multiple of $2\pi/\beta$. This does not necessarily imply a similar property for each individual $\kappa_i = \kappa_f(\epsilon_i)$, however values close to multiples of $2\pi/\beta$ are generally taken.

We see this most easily for the case $\kappa_1 = -\kappa_2$, i.e. $\theta_1 = -\theta_2$. The quantization condition (18) for y_0 requires $y_0 = \infty$. If we apply the (1OA) treatment to (16), the quantization condition (18) simply reads $\ln a(\theta_i + i\gamma/2) = i\beta v/\sinh(\pi/\gamma)\theta_i = $ odd multiple of πi. Using this when inserting (22) into (11) we directly find $\kappa_1 = -k_2 = 2\pi/\beta$.

If both κ_1 and κ_2 take the smallest possible values of same sign and the XXZ chain is in the attractive regime $\pi/2 \leq \gamma < \pi$ the quantization conditions impose complex values for the parameters $\theta_{1,2}$. This leads us to the study of bound states of the QTM.

Bound States

Here we content ourselves to a motivation of why in the attractive regime complex solutions to (18) close to

$$\theta_{1,2} = \theta \pm i\left(\gamma - \frac{\pi}{2}\right), \tag{25}$$

appear. To this end let us assume that θ_1 has a positive imaginary part and we calculate $\ln a(\theta_1 + i\gamma/2)$ from (16). For low temperatures the dominant term is $-\beta v/\cosh(\pi/\gamma)(\theta_1 + i\gamma/2)$ whose real part tends to $+\infty$ in the limit $\beta \to \infty$. The only term matching this divergence is the y_0 term in the first line of (16) if $\theta_1 - y_0 = \gamma - \pi$. Likewise we conclude for θ_2 with negative imaginary part the condition $\theta_2 - y_0 + \gamma = 0$. Using $\mathrm{Im}y_0 = \pi/2$ we write $y_0 = \theta + i\pi/2$ and arrive at (25).

We like to note that for the case of higher-lying states involving more than one complex rapidity y_0 there are additional bound states. These always involve two complex conjugate parameters $\theta_{1,2}$ and a "string" of complex rapidities y_j with minimum number 1 and maximum number $[\gamma/(\pi - \gamma)]$, a situation similar to that of the Hamiltonian. However, for the crossover phenomenon in the correlation functions the case explicitly studied above is sufficient.

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The momentum-energy dispersion is obtained from (22,25) inserted into (11) and eliminating θ. More easily we may use the relation to (6) $\kappa_b(\epsilon) = -i\epsilon_b(i\epsilon)$. With $\mu = 1$ we find

$$\kappa_b(\epsilon) = \pm v\, 2\sinh\frac{\epsilon}{2}\sqrt{1 - a^2\sinh^2\frac{\epsilon}{2}}, \qquad a = \cot\left(\frac{\pi - \gamma}{\gamma}\frac{\pi}{2}\right). \qquad (26)$$

4 Crossover Phenomena

In this section we are going to investigate various crossover phenomena in correlation functions as well as macroscopic properties of the XXZ chain in the attractive regime. Of prime interest is the calculation of the crossover temperature as function of the anisotropy parameter $-1 < \Delta \leq 0$.

4.1 Crossover in Correlation Functions

With the knowledge of Sec. 3.4 we are in the position to examine the crossover of the asymptotics of the longitudinal correlation function from ferromagnetic behaviour at high temperature to antiferromagnetic behaviour at low temperature. In particular we want to derive an analytic formula for the crossover temperature as function of the anisotropy Δ. In principle such a crossover may occur under two separate circumstances

- (i) the prefactor A_1 of the dominant term in (9), i.e. that with longest correlation length $\xi_1 = 1/(\mathcal{E}_1 - \mathcal{E}_0)$, turns zero for some temperature.

- (ii) the leading and next-leading terms in (9) have prefactors A_1 and A_2 of different sign, and a crossover of the correlation lengths ξ_1 and ξ_2 occurs for some temperature.

Unfortunately, we cannot calculate the prefactors as matrix elements are currently out of reach of our formalism. In the work[10] scenario (i) was advocated, because it naturally leads to a crossover for $\langle \sigma_0^Z \sigma_n^Z \rangle$ at a temperature $T_0(n)$ which in dependence on the separation n converges to T_0 with exponential rate (formula (2.10) of [10] with three fit parameters). For scenario (ii) the dependence of $T_0(n)$ would be algebraic $T_0 + A/n$ with two fit parameters T_0 and A. In fact, the exponential fit looks more convincing than the algebraic fit. However, the latter procedure involves one fit parameter less.

As the implications of the fit procedures are not conclusive we performed a numerical study of the QTM for finite N which already allows for quite accurate, non-trivial high temperature investigations for values of Δ close to 0. Surprisingly, this exercise having been aimed at discriminating between the

two scenarios showed for $N = 4$ that actually *both* take place at the *same* temperature! However, for $N = 6$ only scenario (ii) is realized. We have performed complete eigenvalue computations for much larger numbers N up to 14 and always find scenario (ii) realized. For these larger numbers of N we have not yet computed the matrix elements such that we cannot decisively comment on (i) at the moment.

In the following we investigate scenario (ii) in detail, i.e. the crossover in the two largest correlation lengths, or equivalently in the corresponding "energies" $\mathcal{E}$ for the lowest state with $\mathcal{K} = 0$ and the two lowest states with $\mathcal{K} = \pm 2\pi/\beta$ which are free and bound states, respectively. Such a level crossing analysis can of course be performed within our approach.

The condition for the crossover of a free state with momenta $\kappa_1 = -\kappa_2 = 2\pi/\beta_0$ and a bound state with momentum $\kappa = 2\pi/\beta_0$ where β_0 corresponds to crossover temperature T_0 is

$$\epsilon = \epsilon_1 + \epsilon_2 \text{ and } 2\kappa = \kappa_1 + \kappa_2$$
$$\Longrightarrow 2 \sinh \epsilon_i \sqrt{1 - a^2 \sinh^2 \epsilon_i} = \sinh \epsilon_i, \qquad (27)$$

with solution $\sinh^2 \epsilon_i = \frac{3}{4a^2}$. Inserting this into $\kappa_f(\epsilon_i) = 2\pi/\beta_0$ yields

$$T_0 = \frac{\sqrt{3}}{4} \frac{\sin \gamma}{\gamma} \tan \left(\frac{\pi - \gamma}{\gamma} \frac{\pi}{2} \right). \qquad (28)$$

This is in excellent agreement with the numerical analysis of [10], see Fig. 1. An almost perfect agreement with the numerical results has been achieved by introducing a multiplicative correction close to 1 and independent of Δ. Of course, some correction term had to be expected as we only calculated within the 1OA.

In addition we show "analytical" results for the nearest-neighbour correlations $\langle \sigma_j^Z \sigma_{j+1}^Z \rangle_{T>0}$ derived as derivatives of the free energy with respect to Δ, see Fig. 2.

4.2 Crossover in Macroscopic Quantities

Finally, we like to present a qualitative argument based on the dispersion relations of the elementary excitations of the Hamiltonian (4,6) to show crossover between ferromagnetic and antiferromagnetic behaviour at high and low temperatures, respectively. Notice that the dispersion of free states (4) is quasislinear, i.e. is approximated well by a linear relation as long as the momentum transfer is less than the reciprocal lattice vector π. For the bound states (6)
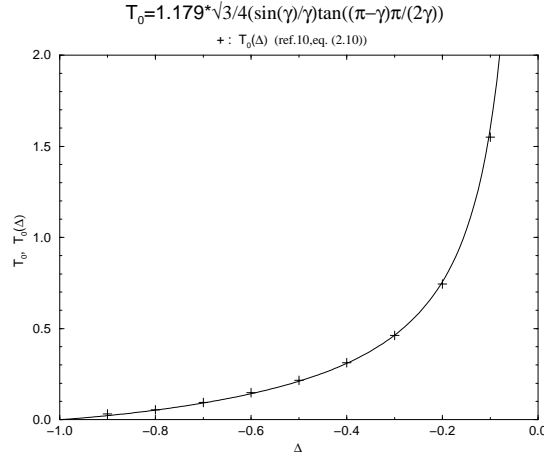
$$T_0 = 1.179 * \sqrt{3/4} (\sin(\gamma)/\gamma) \tan((\pi-\gamma)\pi/(2\gamma))$$

$+: \ T_0(\Delta) \ \text{(ref.10,eq. (2.10))}$

Figure 1: Dependence of the crossover temperature T_0 as function of Δ. Crosses denote numerical values, the solid line corresponds to the analytic result (28) where a scale factor 1.179 independent of Δ has been introduced.
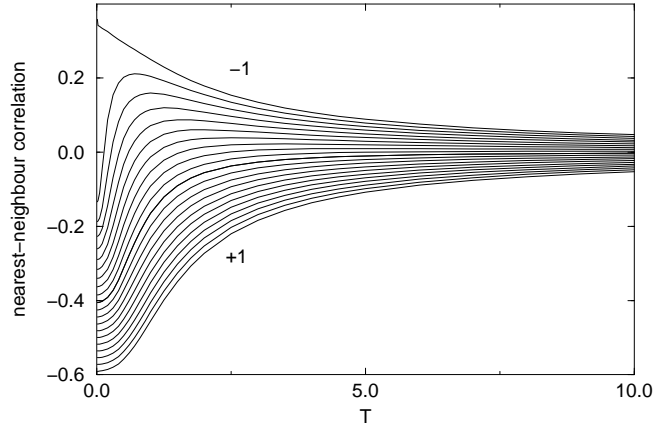

Figure 2: Temperature dependence of the nearest-neighbour correlation $\langle \sigma_j^Z \sigma_{j+1}^Z \rangle$ for $\Delta = -1, -0.9, ..., 0.9, 1.0$. Note that for $0 \leq \Delta \leq 1$ and all temperatures the values are negative. For $-1 < \Delta < 0$ there is a crossover from positive to negative values when passing from high to low temperatures. For $\Delta = -1$ and all temperatures the correlation takes positive values which in the limit $T = 0$ should approach the value $+1$ in a singular manner.
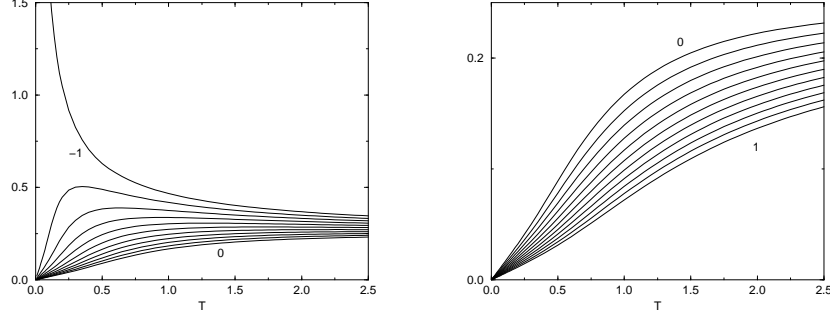
11

Figure 3: Depiction of $\chi(T) \cdot T = \sum_j \langle S_0^Z S_{j+1}^Z \rangle$ for (a) $\Delta = -1, -0.9, ..., 0$ and (b) $\Delta = 0, 0.1, ..., 1$. Note the existence of maxima of $\chi(T) \cdot T$ at temperatures of the order T_0' for the attractive case (a). No maxima are observed in the repulsive case (b).

the linear regime is much smaller. For $0 < k < (\pi - \gamma)\pi/2\gamma$ the dispersion behaves like $\epsilon_b(k) \simeq v \, 2 \sin \frac{k}{2}$, i.e. it is quasi-linear. For $(\pi - \gamma)\pi/2\gamma < k < \pi$ we find the dependence $\epsilon_b(k) \simeq v \, 2a \sin^2 k/2$, i.e. quadratic behaviour typical for the elementary excitations of an isotropic ferromagnetic system. The crossover takes place for $a \sin k_c/2 = 1$ with crossover temperature

$$T_0' = \epsilon_b(k_c) = 2^{3/2} v/a = 2^{3/2} \pi \frac{\sin \gamma}{\gamma} \tan \left(\frac{\pi - \gamma}{\gamma} \frac{\pi}{2} \right). \qquad (29)$$

Note that T_0' is larger than T_0 by a factor of 20.52..., though the functional dependence on Δ is identical. We see that both arguments (crossover of free and bound states of the QTM, and crossover from linear to quadratic dispersion of the bound states of the Hamiltonian) share the same physical origin, but apply to different properties. In fact, at temperatures of the order T_0' we see characteristics in the susceptibility data which do not exist for the repulsive regime $0 < \Delta < 1$, see Fig. 3. For any $-1 < \Delta$ we have $\lim_{T \to 0} \chi(T) \cdot T = 0$, whereas for $\Delta = -1$ the result is divergent, $\chi(T) \simeq J/(6T^2)$, see [19,20]. The noncontinuity of the limiting values is the reason for the observed temperature maximum of the quantity $\chi(T) \cdot T$.

For completeness we show results for the specific heat of the XXZ chain in the attractive as well as repulsive regime. Note there are no characteristics like finite temperature maxima in $c(T)$ in addition to the usual "peak" typical for spin systems with a finite number of degrees per lattice site.
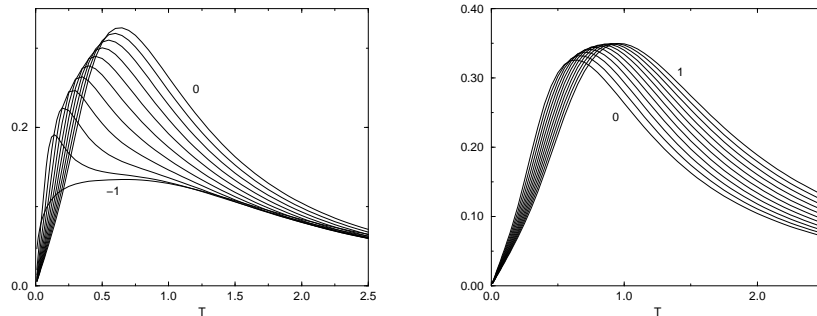
Figure 4: Depiction of $c(T)$ for (a) $\Delta = -1, -0.9, ..., 0$ and (b) $\Delta = 0, 0.1, ..., 1$.

5 Conclusion

We have studied the competition of ferromagnetic and antiferromagnetic order in the longitudinal correlation function of the spin-1/2 XXZ chain in the attractive regime. Within the scenario of level crossing of the quantum transfer matrix we found an explanation of the sign change in the dominant exponential asymptotics from positive to negative values when passing from high to low temperatures. Notably, we found an analytic formula for the crossover temperature $T_0(\Delta)$ (28) as function of $-1 < \Delta < 0$ which may be viewed as the maximum temperature below which conformal field theory is applicable. The agreement of T_0 as determined numerically and analytically is very good.

The physical origin underlying the crossover phenomena in correlation functions (as well as the magnetic susceptibility) may be viewed in the existence of bound states. The various manifestations of these peculiar properties of the spectrum of the quantum transfer matrix (as well as the Hamiltonian) have been discussed. A lesson to be drawn from these findings is that the physical properties of systems possessing bound states are much richer than the usual low-energy treatment within bosonization and a subsequent approximation by Gaussian models.

We want to point out two important questions which remained unanswered. First, for the explanation of the crossover there are two different scenarios conceivable. For the numerical analysis a sign change of the coefficient A_1 of the leading term in (9) was assumed [10], the analytical work in this paper was based on a level crossing scenario as also found in explicit numerical treatments of QTMs for Trotter numbers $4 \leq N \leq 14$. The new level crossing

scenario would suggest a numerical size analysis of the crossover temperature somewhat different from that employed in [10]. In preliminary numerical work we have seen this change to affect the numerical value of the crossover temperature T_0 in only about the second significant digit. In our future work we want to focus on a numerical analysis of the Hamiltonian [10] and the QTM approach (to be published) yielding identical numerical values for T_0.

Second, even within the level crossing scenario of our analytic reasoning the result (28) represents an analytic approximation to the characteristic temperature T_0. A comprehensive numerical treatment of (15,16) beyond the (1OA) approximation is on the way.

As a result of the analytical and numerical computations of finite N–QTM's we expect a decisive answer to the open problems.

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